Upper bounds on the size of 4- and 6-cycle-free subgraphs of the hypercube

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Abstract

In this paper we modify slightly Razborov's flag algebras machinery to be suitable for the hypercube. We use this modified method to show that the maximum number of edges of a 4-cycle-free subgraph of the n-dimensional hypercube is at most 0.6068 times the number of its edges. We also improve the upper bound on the number of edges for 6-cycle-free subgraphs of the n-dimensional hypercube from $\sqrt{2}-1$ to 0.3755 times the number of its edges. Additionally, we show that if the n-dimensional hypercube is considered as a poset then the maximum vertex density of three middle layers in an induced subgraph without 4-cycles is at most $2.15121\binom{n}{\lfloor n/2 \rfloor}$.

1 Introduction

Let $\mathcal{Q}_n$ be the graph of the n-dimensional hypercube (n-cube) whose vertex set is the set $\{0,1\}^n$ of binary n-tuples, and two vertices are adjacent if and only if they differ in exactly one coordinate. The *Hamming distance* between two n-tuples u and v, denoted by $d(u,v)$, is the number of coordinates in which they differ. So uv is an edge of $\mathcal{Q}_n$ if and only if $d(u,v)=1$. Note that the hypercube $\mathcal{Q}_n$ has 2^n vertices and $n2^{n-1}$ edges.

Let $e(G)$ denote the number of edges of a graph G. For a graph F, we define $\mathrm{ex}_{\mathcal{Q}}(n,F)$ to be the maximum number of edges of an F-free subgraph of $\mathcal{Q}_n$ and define

$$\pi_{\mathcal{Q}}(F) = \lim_{n\to\infty} \frac{\mathrm{ex}_{\mathcal{Q}}(n,F)}{e(\mathcal{Q}_n)}.$$

Note that the existence of the limit follows from an easy averaging argument that $\mathrm{ex}_{\mathcal{Q}}(n,F)/e(\mathcal{Q}_n)$ is non-increasing as n increases.

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Erdős [12, 13] was the first one who considered Turán type problems for the hypercube. He proposed a problem of determining $\mathrm{ex}_{\mathcal{Q}}(n, C_{2t})$, suggesting that for all $t > 2$ perhaps $o(e(\mathcal{Q}_n))$ was an upper bound. It turned out to be false for $t = 3$ as Chung [9] and Brouwer, Dejter and Thomassen [8] found a 4-coloring of the hypercube without a monochromatic C_6. This was later improved by Conder [10] to a 3-coloring. This implies that $\mathrm{ex}_{\mathcal{Q}}(n, C_6) \geq \frac{1}{3}e(\mathcal{Q}_n)$. On the other hand, the best known upper bound obtained by Chung [9] is $\mathrm{ex}_{\mathcal{Q}}(n, C_6) \leq (\sqrt{2} - 1 + o(1))e(\mathcal{Q}_n)$.

Chung [9] also showed that Erdős was right for even $t \geq 4$ by proving that $\mathrm{ex}_{\mathcal{Q}}(n, C_{2t}) = o(e(\mathcal{Q}_n))$. Füredi and Özkahya [15, 16] complemented the previous result by showing that $\mathrm{ex}_{\mathcal{Q}}(n, C_{2t}) = o(e(\mathcal{Q}_n))$ for all odd $t \geq 7$. Their approaches were recently unified by Conlon [11]. Despite the efforts in [1, 3, 11] the case $\mathrm{ex}_{\mathcal{Q}}(n, C_{10})$ still remains unsolved.

Erdős [12] was particularly interested in $\mathrm{ex}_{\mathcal{Q}}(n, C_4)$. He conjectured that the answer is $\pi_{\mathcal{Q}}(C_4) = 1/2$ and offered \$100 for a solution. Best known lower bound $\frac{1}{2}(1+\frac{1}{\sqrt{n}})e(\mathcal{Q}_n)$ (valid when n is a power of 4) on $\mathrm{ex}_{\mathcal{Q}}(n, C_4)$ was obtained by Brass, Harborth and Nienborg [7]. The upper bound on $\pi_{\mathcal{Q}}(C_4)$ of 0.62284 obtained by Chung [9] was recently improved by Thomason and Wagner [24] by a computer assisted proof to 0.62256. They also claimed that $\pi_{\mathcal{Q}}(C_4) \leq 0.62083$ can be obtained with the same technique.

Razborov [23] developed a systematic approach to bound densities of subgraphs called flag algebras. This method can be applied to various problems [17, 18, 19, 20]. One nice exposition of applying the method to Turán density is in [5], for a recent development see [14]. We present a modification of the method for subgraphs of the hypercube. By applying our modified flag algebra method we obtained improvements on the upper bounds on $\pi_{\mathcal{Q}}(C_4)$ and $\pi_{\mathcal{Q}}(C_6)$.

Theorem 1. $\pi_{\mathcal{Q}}(C_4) \leq 0.6068$.

Theorem 2. $\pi_{\mathcal{Q}}(C_6) \leq 0.3755$.

These results were independently proved by Baber [4] which originally appeared in his PhD thesis in March 2011. Let us note that although the results are the same, we use a different way of defining flag algebras for hypercubes. Baber is using colored hypercubes while we use subgaphs. Our method is slightly more general since it allows considering subgraphs which are not hypercubes. Baber also estimated vertex Turán density of $\mathcal{Q}_3$ and determined vertex Turán density of $\mathcal{Q}_3$ with one vertex removed for hypercubes.

Both proofs are computer assisted as the number of considered cases is too large to be computed by hand without an extreme suffering (of students and a postdoc). All the programs as well as their inputs and outputs can be obtained at `http://www.math.uiuc.edu/~jobal/cikk/hypercube`.

In addition to spanning subgraphs of the hypercube, flag algebras can be used also for induced subgraphs of the hypercube. However, we present the result in a lattice settings because of its original motivation. For a family F of subsets of $[n] = \{1, 2, \ldots, n\}$ ordered by inclusion, and a partially ordered set P, we say that F is P-free if it does not contain a subposet isomorphic to P. Let $\mathrm{ex}(n, P)$ be the largest size of a P-free family of subsets of $[n]$.

Let Q_2 be the poset with distinct elements a, b, c, d where $a < b, c < d$; i.e., the 2-dimensional Boolean lattice. Axenovich, Manske and Martin [2] showed that $2N - o(N) \leq \mathrm{ex}(n, Q_2) \leq 2.283261N + o(N)$ where $N = \binom{n}{\lfloor n/2 \rfloor}$. It was recently improved by Kramer, Martin and Young [21] to $2.25N + o(N)$. Axenovich et. al. [2] also proved that the largest Q_2-free family of subsets of $[n]$ having at most three different sizes has at most $(3+\sqrt{2})N/2 + o(N)$ members. This was further improved by Manske and Shen [22] to $(3+2\sqrt{3})N/3 + o(N) \approx 2.1547N + o(N)$. This result can be further improved by using flag algebras. We show how to achieve the same bound $(3+\sqrt{2})N/2$ that can be verified by hand. With help of computers we then improve the bound to $2.15121N$.

Theorem 3. *The largest Q_2-free family of subsets of $[n]$ having at most three different sizes has at most $2.15121N$ members where $N = \binom{n}{\lfloor n/2 \rfloor}$.*

In the next section we give a brief introduction to the flag algebra method and describe our modification of it to subgraphs of the hypercube. We refer the interested reader to the seminal paper of Razborov [23] for a detailed exposition of the method. In Section 3 we apply the method with a simple setting and obtain an upper bound $\pi_{\mathcal{Q}}(C_4) \leq 2/3$. The main purpose of Section 3 is to make the reader comfortable with the terminology and describe the proof technique. Finally, in Sections 4 and 5 we give ideas of the proofs of Theorems 1 and 2, respectively. We do not include all the technicalities of the proofs as the number of considered graphs is too large. The interested reader may see all the technical details at `http://www.math.uiuc.edu/~jobal/cikk/hypercube`. The last section is devoted to giving a proof idea of Theorem 3.

2 The flag algebra method for the hypercube

In this section we give a brief introduction to the flag algebra method mixed with the necessary modifications for subgraphs of the hypercube. We say that a graph G is a *cube graph* if G is a subgraph of $\mathcal{Q}_n$ for some n, so $V(G) \subseteq \{0,1\}^n$ and if uv is an edge of G then $d(u,v) = 1$.

Given a cube graph G and a subset U of $V(G)$, we denote the subgraph of G induced by U by $G[U]$. It is easy to see that $G[U]$ is also a cube graph.

Given a subset U of $\{0,1\}^n$, let $D(U)$ be the set of coordinates i such that there exist $v, w \in U$ which differ in the coordinate i (v and w may differ in more coordinates). If $U = \{u, v\}$, then we abbreviate $D(\{u,v\})$ to $D(u,v)$. Let $d(U) = |D(U)|$ and again $d(\{u,v\})$ is abbreviated to $d(u,v)$, as it is the Hamming distance of u and v. We define the *dimension* of a cube graph G to be $\dim(G) = d(V(G))$. Given a vertex $v \in \{0,1\}^n$, let $v[i]$ be its i^{th} coordinate. Given a vertex set $U \subseteq \{0,1\}^n$ of dimension r, let $Q(U)$ be the set of vertices of the unique r-cube containing U, i.e.

$$Q(U) = \{v : v \in \{0,1\}^n, \forall u \in U, i \notin D(U), v[i] = u[i]\}.$$

Given $V \subseteq \{0,1\}^m$ and $U \subseteq \{0,1\}^n$, we say a map $f : V \to U$ is *Hamming distance preserving* if $\forall u, v \in V, d(u,v) = d(f(u), f(v))$. Note that a Hamming distance preserving map is injective since $d(u,v) = 0$ iff $u = v$. When $U = V = \{0,1\}^n$, such f is a *cube automorphism.* We call a map $f : V \to U$ *feasible* if there exists a Hamming distance preserving map $\tilde{f} : Q(V) \to Q(U)$ such that $f(v) = \tilde{f}(v)$ for all $v \in V$. Given two cube graphs H and G, we say H and G are *feasible isomorphic* (denoted by $H \simeq G$) if there exists a feasible bijection $f : V(H) \to V(G)$ satisfying $\forall u, v \in V(H), f(u)f(v) \in E(G)$ iff $uv \in E(H)$. Such f is called a *feasible isomorphism* from H to G. See Figure 1 for an example.

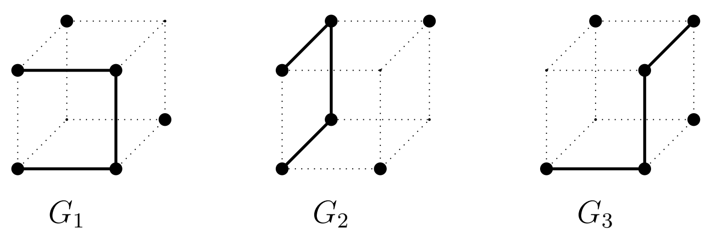

Figure 1: All G_1, G_2 and G_3 are isomorphic. However, only G_1 and G_2 are feasible isomorphic.

It is not hard to see that a feasible map preserves the dimension. Indeed, we have a stronger statement.

Lemma 1. *Let $V \subseteq \{0,1\}^m, U \subseteq \{0,1\}^n$ and let $f : V \to U$ be a feasible map. Then there exists an injective map $\phi : D(V) \to D(U)$ such that for any subset $V' \subseteq V$, we have $D(f(V')) = \phi(D(V'))$. Given ϕ and $f(v)$ for any $v \in V$, then f is uniquely determined.*

Proof. As f is feasible, there exists a Hamming distance preserving map $\tilde{f} : Q(V) \to Q(U)$ such that $f(v) = \tilde{f}(v)$ for every $v \in V$. We start by inspecting $\tilde{f}$. Let $d(V) = k$ and $D(V) = \{l_1, \ldots, l_k\}$. Pick a vertex $v \in V$ and let $v_i \in Q(V)$ be the vertex which differs from v only in the coordinate l_i. As $\tilde{f}$ is Hamming distance preserving, $\tilde{f}(v_i)$ differs from $\tilde{f}(v)$ in only one coordinate, say l'_i. Then we have $l'_i \neq l'_j$ for $i \neq j$ since $\tilde{f}$ is injective. Next we define $\phi(l_i) = l'_i$ for all $1 \leq i \leq k$ and show that it satisfies our needs. Because $\tilde{f}$ is Hamming distance preserving, for a vertex $u \in Q(V)$ we have $D(\tilde{f}(u), \tilde{f}(v)) = \phi(D(u,v))$, which means f is uniquely determined by ϕ and $f(v)$. Furthermore, for any two vertices $v_1, v_2 \in Q(V)$ we have $D(\tilde{f}(v_1), \tilde{f}(v_2)) = \phi(D(v_1, v_2))$ since

$$D(\tilde{f}(v_1), \tilde{f}(v_2)) = D(\tilde{f}(v), \tilde{f}(v_1)) \triangle D(\tilde{f}(v), \tilde{f}(v_2))$$

and $\phi(D(v_1, v_2)) = \phi(D(v, v_1)) \triangle \phi(D(v, v_2))$, where $\triangle$ means the symmetric difference of the sets. Then for any subset $V' \subseteq V$, we have $D(f(V')) = \phi(D(V'))$. $\square$

Let F be a fixed graph. Our goal is to compute an upper bound on $\pi_{\mathcal{Q}}(F)$. Let $\mathcal{H}_s$ be the family of all F-free spanning subgraphs of $\mathcal{Q}_s$, up to cube automorphism.

Given any two cube graphs H and G, we define $p(H,G)$ to be the probability that a feasible map $f : V(H) \to V(G)$ chosen uniformly at random satisfies $G[Im(f)] \simeq H$. Note that if $H \in \mathcal{H}_s$ and $V(G) = V(\mathcal{Q}_n)$ then $\mathcal{Q}_n[Im(f)] \simeq \mathcal{Q}_s$.

Given a cube graph G, let $n = \dim(G)$, then define its edge density $\rho(G) = e(G)/e(\mathcal{Q}_n)$. Let G be an F-free spanning subgraph of $\mathcal{Q}_n$. By averaging over all $H \in \mathcal{H}_s$ we have

$$\rho(G) = \sum_{H \in \mathcal{H}_s} \rho(H) p(H,G) \tag{1}$$

as $\sum_{H \in \mathcal{H}_s} p(H,G) = 1$. Hence $\rho(G) \le \max_{H \in \mathcal{H}_s} \rho(H)$ and then $\pi_{\mathcal{Q}}(F) \le \max_{H \in \mathcal{H}_s} \rho(H)$.

This bound in general is very poor, for $F = C_4$ and $s \in \{2,3,4\}$ it gives that $\pi_{\mathcal{Q}}(F) \le 3/4$. It is because this bound only considers $\rho(H)$. It does not use other structural properties of graphs in $\mathcal{H}_s$. Razborov's flag algebra method allows us to make use of more information about $\mathcal{H}_s$ and hence it gives a much better bound. Indeed, our results are obtained with $s = 3$.

Let H be a cube graph, we call an injective map $\theta : [m] \to V(H)$ a *type map to H* if every vertex $v \in V(H) \setminus Im(\theta)$ satisfies $v \notin Q(Im(\theta))$. A *flag* (H,θ) is H together with a type map θ. If θ is also bijective, then we call the flag a *type*. We can think of θ as a labeling. If $m = 0$, then no vertex is labeled, and we use 0 to denote such type. Let $F_1 = (H,\theta)$ be a flag. We say F_1 is *F-free* if H is F-free. We say F_1 is a *σ-flag* if $(Im(\theta),\theta) \simeq \sigma$. See Figure 2 for examples. Let H_1, H_2 be two cube graphs. We call two flags $F_1 = (H_1,\theta_1)$ and $F_2 = (H_2,\theta_2)$ *isomorphic* (denoted by $F_1 \simeq F_2$) if there exists a feasible isomorphism $f : V(H_1) \to V(H_2)$ satisfying $f \cdot \theta_1 = \theta_2$.

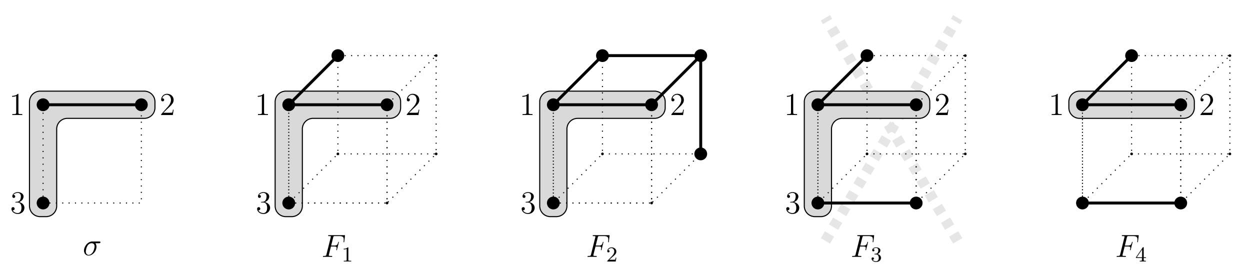

Figure 2: σ is a type, F_1 and F_2 are σ-flags but F_3 is not a flag. It contains an unlabeled vertex in $Q(Im(\theta))$. F_4 is a flag but not a σ-flag as the labeled vertices do not induce σ.

Let σ be a type of dimension r. Let G be a (large) F-free spanning subgraph of $\mathcal{Q}_n$, so $\dim(G) = n$. We say a type map θ to G is a *σ-type map* if there exists a feasible bijection $f : Im(\theta) \to V(\sigma)$. Let Θ be the set of all σ-type maps θ to G. Let $\mathcal{F}_k^\sigma$ be the set of all F-free σ-flags of dimension k. Given a σ-flag $F_1 = (H_1,\theta_1) \in \mathcal{F}_k^\sigma$ and a map $\theta \in \Theta$, we define $p(F_1,\theta;G)$ to be the probability that a feasible map $f : V(H_1) \to V(G)$ chosen uniformly at random subject to $f \cdot \theta_1 = \theta$ satisfies $(G[Im(f)],\theta) \simeq F_1$. Note that if $(Im(\theta),\theta) \not\simeq \sigma$, then $p(F_1,\theta;G)=0$. Given two σ-flags $F_1=(H_1,\theta_1)\in\mathcal{F}^{\sigma}_{k_1}$ and $F_2=(H_2,\theta_2)\in\mathcal{F}^{\sigma}_{k_2}$, for $\theta\in\Theta$, we define $p(F_1,F_2,\theta;G)$ to be the probability that if we choose two feasible maps $f_1:V(H_1)\to V(G)$ and $f_2:V(H_2)\to V(G)$ uniformly and independently at random subject to $f_1\cdot\theta_1=\theta$, $f_2\cdot\theta_2=\theta$ and $D(Im(f_1))\cap D(Im(f_2))=D(Im(\theta))$, then

$$(G[Im(f_1)],\theta)\simeq F_1 \text{ and } (G[Im(f_2)],\theta)\simeq F_2.$$

Note that $p(F_1,F_2,\theta;G)$ makes sense only when $n\geq k_1+k_2-r$ since $D\left(Im(f_1)\cup Im(f_2)\right)=D(Im(f_1))\cup D(Im(f_2))$ must be a subset of $D(V(G))$. When comparing $p(F_1,F_2,\theta;G)$ with $p(F_1,\theta;G)p(F_2,\theta;G)$, we see that the only difference between these two probabilities is that in $p(F_1,\theta;G)p(F_2,\theta;G)$ we ask only for

$$f_1\cdot\theta_1=\theta \text{ and } f_2\cdot\theta_2=\theta \tag{2}$$

where f_1,f_2 are two randomly chosen feasible maps, while in $p(F_1,F_2,\theta;G)$ we ask not only for (2) but also for

$$D(Im(\theta))=D(Im(f_1))\cap D(Im(f_2)). \tag{3}$$

When n is very large, intuitively, if (2) holds, then with high probability (3) also holds, and then the difference between these two probabilities is negligible. This following lemma states it formally. It is similar to Lemma 2.1 in [5], which is a special case of Lemma 2.3 in [23].

Lemma 2. *For any $F_1=(H_1,\theta_1)\in\mathcal{F}^{\sigma}_{k_1}$, $F_2=(H_2,\theta_2)\in\mathcal{F}^{\sigma}_{k_2}$, $\theta\in\Theta$, and G being a spanning subgraph of $\mathcal{Q}_n$ it holds that*

$$p(F_1,\theta;G)p(F_2,\theta;G)=p(F_1,F_2,\theta;G)+o(1)$$

where the $o(1)$ term tends to 0 as n tends to infinity.

Proof. Choose two independent feasible maps $f_1:V(H_1)\to V(G)$ and $f_2:V(H_2)\to V(G)$ uniformly at random subject to $f_1\cdot\theta_1=\theta$ and $f_2\cdot\theta_2=\theta$. For such choices of f_1 and f_2, let A be the event

$$(G[Im(f_1)],\theta)\simeq F_1 \text{ and } (G[Im(f_2)],\theta)\simeq F_2,$$

and B be the event

$$D(Im(f_1))\cap D(Im(f_2))=D(Im(\theta)).$$

We have $p(F_1,\theta;G)p(F_2,\theta;G)=P(A)$ and $p(F_1,F_2,\theta;G)=P(A|B)$. Using that for any A and B, it holds that

$$P(A|B)P(B)=P(A\cap B)\leq P(A)\leq P(A\cap B)+P(\overline{B}),$$

we have $|P(A|B)P(B)-P(A)|\leq P(\overline{B})$. Hence it suffices to show $P(B)\geq 1-o(1)$. Note that $P(B)$ depends on $V(H_1),V(H_2),V(G)$ but not on the edges of these graphs.

For $i=1,2$, let ϕ_i be the ϕ in Lemma 1 for f_i. We compute $P(B)$ by counting possible choices of ϕ_i instead of counting f_i's directly. We first consider the case that the type $\sigma\neq 0$, i.e., some vertex is labeled. From $f_i \cdot \theta_i = \theta$ we know that $\phi_i(D(Im(\theta_i))) = D(Im(\theta))$, so we next need to look at ϕ_i on $D(V(H_i)) \setminus D(Im(\theta_i))$. Recall that $d(Im(\theta)) = r$, hence there are still $k_i - r$ coordinates to be chosen from $[n] \setminus D(Im(\theta))$.

We know $f_i(\theta_i(1)) = \theta(1)$, so each ϕ_i gives one feasible map f_i. Note that different choices of ϕ_i may give the same f_i. Let M_i be the number of feasible maps $f_i' : V(H_i) \to Q\left(V(H_i)\right)$ satisfying $f_i' \cdot \theta_i = \theta_i$. Observe that M_i is also the number of f_i's for each choice of $(k_i - r)$ coordinates from $[n] \setminus D(Im(\theta))$ given that $f_i \cdot \theta_i = \theta$. Note that good choices for the event B are choosing coordinates for $\phi_1(D(V(H_1)) \setminus D(Im(\theta_1)))$ and $\phi_2(D(V(H_2)) \setminus D(Im(\theta_2)))$ that are disjoint. So we can compute that

$$P(B) = \frac{\binom{n-r}{k_1-r} M_1 \binom{n-k_1}{k_2-r} M_2}{\binom{n-r}{k_1-r} M_1 \binom{n-r}{k_2-r} M_2} = 1 - o(1).$$

For the case $\sigma = 0$, each choice of ϕ_i will give 2^n different f_i's, so we have

$$P(B) = \frac{\binom{n}{k_1} M_1 2^n \binom{n-k_1}{k_2} M_2 2^n}{\binom{n}{k_1} M_1 2^n \binom{n}{k_2} M_2 2^n} = 1 - o(1).$$

□

Now we can use this version of the flag algebra method to compute $\mathrm{ex}_{\mathcal{Q}}(F)$. This is the same as in [5]. We suggest the reader to start reading the next section in parallel with the following text as the entire next section can be viewed as an example.

Fix a type $\sigma \neq 0$. Averaging over a uniformly and randomly chosen $\theta \in \Theta$ we have

$$\mathbb{E}_{\theta\in\Theta}[p(F_1, \theta; G)p(F_2, \theta; G)] = \mathbb{E}_{\theta\in\Theta}[p(F_1, F_2, \theta; G)] + o(1). \tag{4}$$

Pick $s \geq k_1 + k_2 - r$. For $H \in \mathcal{H}_s$, let Θ_H be the set of all σ-type maps to H. Then

$$\mathbb{E}_{\theta\in\Theta}[p(F_1, F_2, \theta; G)] = \sum_{H\in\mathcal{H}_s} \mathbb{E}_{\theta\in\Theta_H}[p(F_1, F_2, \theta; H)]p(H, G). \tag{5}$$

We pick $\sigma \neq 0$ simply because if $\sigma = 0$, then (5) does not hold. Let $\mathcal{F} = \{F_1, \ldots, F_\ell\} \subseteq \mathcal{F}_k^\sigma$ be satisfying

$$s \geq 2k - r \tag{6}$$

and let $M = (m_{ij})$ be a positive semidefinite ℓ-by-ℓ matrix. For $\theta \in \Theta$ define $\mathbf{p}_\theta = \{p(F_1, \theta; G), \ldots, p(F_\ell, \theta; G)\}$. Using (4) and (5), we have

$$0 \leq \mathbb{E}_{\theta\in\Theta}[\mathbf{p}_\theta M \mathbf{p}_\theta^T] = \sum_{1\leq i,j\leq \ell} \sum_{H\in\mathcal{H}_s} m_{ij} \mathbb{E}_{\theta\in\Theta_H}[p(F_i, F_j, \theta; H)]p(H, G) + o(1). \tag{7}$$

For $H \in \mathcal{H}_s$ we define $c_H(\sigma, \mathcal{F}, M)$ to be the coefficient of $p(H, G)$ in (7) i.e.,

$$c_H(\sigma, \mathcal{F}, M) = \sum_{1\leq i,j\leq \ell} m_{ij} \mathbb{E}_{\theta\in\Theta_H}[p(F_i, F_j, \theta; H)].$$

Then we can rewrite (7) as

$$0 \leq \sum_{H \in \mathcal{H}_s} c_H(\sigma, \mathcal{F}, M) p(H, G) + o(1).$$

Fix G and $\mathcal{H}_s$, suppose we have t choices of $(\sigma_i, \mathcal{F}_i, M_i)$, where each $\sigma_i \neq 0$ is a type of dimension r_i, each $\mathcal{F}_i$ is a subset of $\mathcal{F}_{k_i}^{\sigma_i}$ satisfying $s \geq 2k_i - r_i$, and each M_i is a positive semidefinite matrix of dimension $|\mathcal{F}_i|$. Then for $H \in \mathcal{H}_s$ we have

$$0 \leq \sum_{H \in \mathcal{H}_s} \left(\sum_{i=1}^{t} c_H(\sigma_i, \mathcal{F}_i, M_i) \right) p(H, G) + o(1).$$

Define $c_H = \sum_{i=1}^{t} c_H(\sigma_i, \mathcal{F}_i, M_i)$, then we have $0 \leq \sum_{H \in \mathcal{H}_s} c_H p(H, G) + o(1)$. Together with (1), we have

$$\rho(G) \leq \sum_{H \in \mathcal{H}_s} (\rho(H) + c_H) p(H, G) + o(1).$$

Thus $\rho(G) \leq \max_{H \in \mathcal{H}_s}(\rho(H) + c_H) + o(1)$ and therefore $\pi_{\mathcal{Q}}(F) \leq \max_{H \in \mathcal{H}_s}(\rho(H) + c_H)$.

3 Example for $\mathcal{Q}_2$

In this section we apply the flag algebra method with $F = C_4$ and $\mathcal{H}_2$. We obtain a weaker bound $\pi_{\mathcal{Q}}(C_4) \leq 2/3$ than in Theorem 1. On the other hand, it allows us to present the proof with all the details and hopefully it makes the reader more comfortable while reading the proofs of Theorems 1 and 2 as the method is the same.

We consider only one type, a single labelled vertex, so its dimension is zero. As flags $\mathcal{F} = \{F_0, F_1\}$ we use both possible flags on two vertices with one labelled vertex and containing 0 and 1 edges, respectively. So they both have dimension one. See Figure 3 for F_0 and F_1.

Figure 3: Two flags of dimension one with one labeled vertex.

Recall that $\mathcal{H}_2$ is the set of all C_4-free subgraphs of $\mathcal{Q}_2$. See Figure 4 for the list of all five of them. Note that the variables corresponding to the previous section are $r = 0, k = 1, s = 2$ and $t = 1$. We can use $\mathcal{H}_2$ because (6) holds.

In order to calculate the coefficients c_H we need to compute $\mathbb{E}_{\theta \in \Theta} p(F_i, F_j, \theta, H)$ for all possible $H \in \mathcal{H}_2$ and $F_i, F_j \in \mathcal{F}$. The values of $\mathbb{E}_{\theta \in \Theta} p(F_i, F_j, \theta, H)$ are given in Table 1.

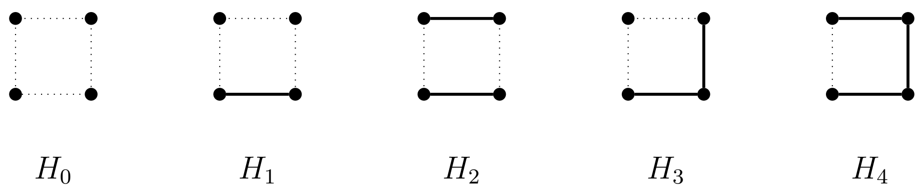

Figure 4: C_4-free spanning subgraphs of $\mathcal{Q}_2$.

	H_0	H_1	H_2	H_3	H_4
F_0, F_0	1	1/2	0	1/4	0
F_0, F_1	0	1/4	1/2	1/4	1/4
F_1, F_1	0	0	0	1/4	1/2

Table 1: $\mathbb{E}_{\theta\in\Theta}p(F_i, F_j, \theta, H)$.

We show how to compute $\mathbb{E}_{\theta\in\Theta}p(F_0, F_1, \theta, H_3)$ and leave the verification of other entries in Table 1 to the interested readers. In this case we need to compute the probability that a uniformly and randomly chosen $\theta \in \Theta$ and two pairs of vertices with Hamming distance one $V_0, V_1 \subset V(H_3)$ chosen independently and uniformly at random with intersection $Im(\theta)$ induce flags $(H_3[V_0], \theta)$ and $(H_3[V_1], \theta)$ that are isomorphic to F_0 and F_1, respectively. By inspection of the cases, this happens only when $Im(\theta)$ is a vertex of degree one and the other vertices of V_0 are V_1 are the vertices of degree zero and two, respectively. So 2 out of 8 possibilities are satisfying the condition.

As $l = 2$, we want to choose a positive semidefinite 2×2 matrix M used in (7). In the general form

$$M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}.$$

Note that $m_{12} = m_{21}$ as M must be symmetric. We can compute $c_H(\sigma, \mathcal{F}, M)$ by multiplying the vector $(m_{11}, 2m_{12}, m_{22})$ with the column corresponding to H in Table 1 for every $H \in \mathcal{H}_2$. Note that $c_H(\sigma, \mathcal{F}, M)$ is the same as c_H because $t = 1$. Together with densities we have

$$\begin{aligned}
\rho(H_0) + c_{H_0} &= 0 + m_{11} \\
\rho(H_1) + c_{H_1} &= 1/4 + m_{11}/2 + m_{12}/2 \\
\rho(H_2) + c_{H_2} &= 1/2 + m_{12} \\
\rho(H_3) + c_{H_3} &= 1/2 + m_{11}/4 + m_{12}/2 + m_{22}/4 \\
\rho(H_4) + c_{H_4} &= 3/4 + m_{12}/2 + m_{22}/2.
\end{aligned}$$

Recall that $\pi_{\mathcal{Q}}(C_4) \leq \max_i(\rho(H_i) + c_{H_i})$. So we want to minimize $\max_i(\rho(H_i) + c_{H_i})$ over all positive semidefinite matrices. This can be expressed as a semidefinite program (P) as follows:

$$(P)\begin{cases}\text{Minimize } v\\ \text{subject to } v \geq \rho(H_i) + c_{H_i}\ \forall H_i \in \mathcal{H}_2\\ v \in \mathbb{R}, M \text{ is positive semidefinite.}\end{cases}$$

The optimal solution of (P) is

$$M^* = \begin{pmatrix} 2/3 & -1/3 \\ -1/3 & 1/6 \end{pmatrix}$$

and it gives $\max_i(\rho(H_i) + c_{H_i}) = 2/3$. Note that it is not necessary to use the optimal solution to get an upper bound but any feasible solution gives an upper bound (of course, not as good the optimal solution). We use this observation later in order to fix rounding errors by CSDP solver.

4 Proof of Theorem 1

The proof of Theorem 1 goes along the same lines as the proof in the previous section. It is just performed with $\mathcal{Q}_3$ and with more flags.

Let $E_0, E_1 \subseteq \mathcal{Q}_1$ be cube graphs with zero and one edge, respectively and let $\theta_i : [2] \to V(E_i)$ for $i \in \{0, 1\}$. We consider two types $\sigma_0 = (E_0, \theta_0)$ and $\sigma_1 = (E_1, \theta_1)$ and flags of dimension two. Let $\mathcal{F}_0 = \{F_0^0, \ldots, F_7^0\}$ be all flags in $\mathcal{F}_2^{\sigma_0}$ on 4 vertices and let $\mathcal{F}_1 = \{F_0^1, \ldots, F_6^1\}$ be all flags in $\mathcal{F}_2^{\sigma_1}$ on 4 vertices. The flag of type σ_1 with four edges is not in $\mathcal{F}_2^{\sigma_1}$ since it is not C_4-free. See Figure 5 for the list of flags.

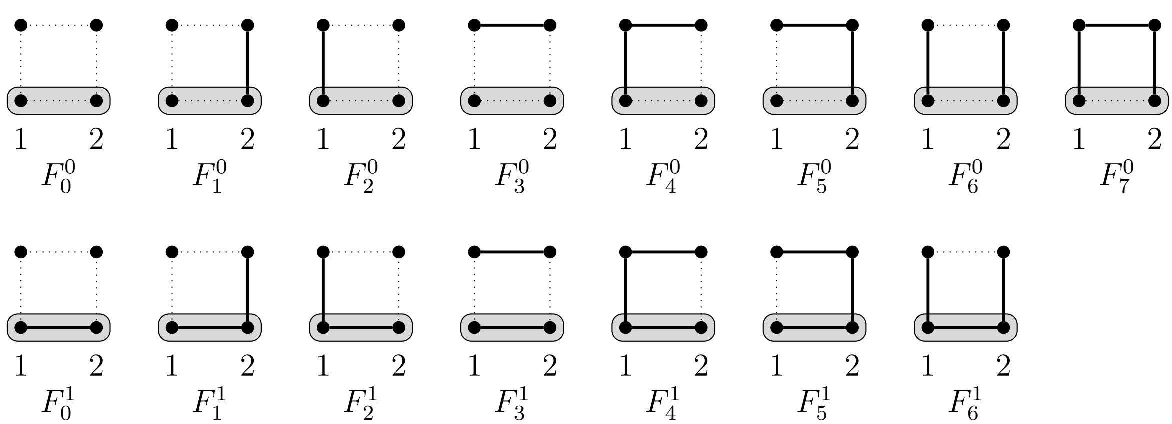

Figure 5: $\mathcal{F}_0$ is in the first row and $\mathcal{F}_1$ is in the second row.

Next we need to obtain $\mathcal{H}_3$, the set of all C_4-free subgraphs of $\mathcal{Q}_3$. We wrote two independent computer programs for generating the graphs and obtained a list of 99 graphs which agrees with [24] where the authors also obtained 99 such graphs.

Our computer programs also calculated $\mathbb{E}_{\theta\in\Theta} p(F_i^k, F_j^k, \theta, H)$ for all possible $H \in \mathcal{H}_3$ and $F_i^k, F_j^k \in \mathcal{F}_k$ and produced a semidefinite program.

The resulting semidefinite program was solved by CSDP [6]. Due to rounding, the resulting matrix M^* may not be positive semidefinite. We used MATLAB to perturb the matrix to make sure that it is positive semidefinite and then we computed an upper bound $\pi_{\mathcal{Q}}(C_4) \leq 0.6068$.

5 Proof of Theorem 2

The proof of Theorem 2 is the same as the proof of Theorem 1. We also considered both types of dimension one with two labeled vertices. In this case we again considered all possible flags on four vertices. See Figure 6 for the list of the flags.

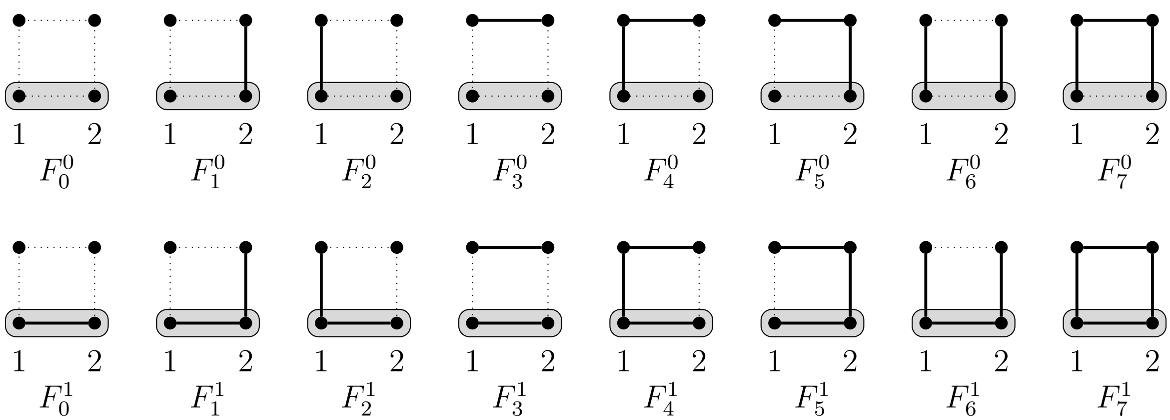

Figure 6: Flags used in the proof of Theorem 2.

Next we need to obtain $\mathcal{H}_3$, the set of all C_6-free subgraphs of $\mathcal{Q}_3$. We wrote two independent computer programs for generating the graphs and obtained a list of 116 graphs. We again used CSDP solver and after perturbation we obtained that $\pi_{\mathcal{Q}}(C_6) \leq 0.3755$.

6 Middle layers

This section describes the idea of proving Theorem 3. We do not give the entire proof as it is computer assisted. Instead, we show a proof of a weaker result which goes along the same way as the proof of Theorem 3. Note that it is easy to see that it is sufficient to show the theorem only for the middle three layers and we are giving an upper bound.

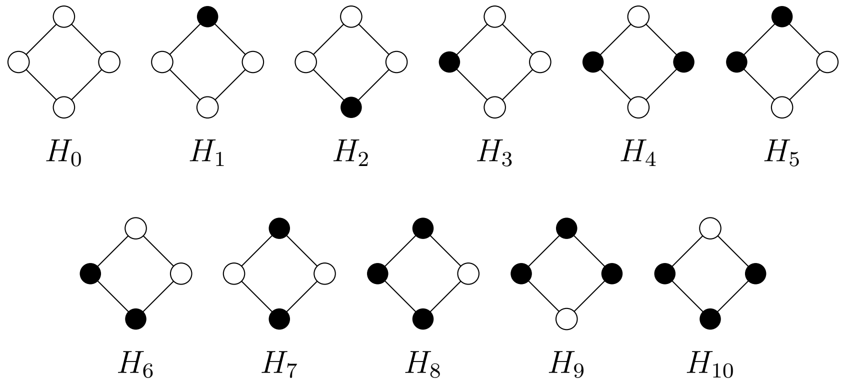

Figure 7: $\mathcal{H}_2$: Q_2-free subsets of M_2.

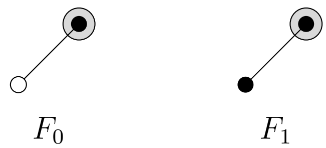

Figure 8: Two flags with one labeled vertex.

We start with describing the upper bound $(3+\sqrt{2})N/2$ using flag algebras. We skip some technical details; namely stating and proving a lemma analogous to Lemma 2 for hypercubes.

Let A_n, B_n, C_n be the family of subsets of $[n]$ having sizes $\lfloor n/2 \rfloor - 1$, $\lfloor n/2 \rfloor$ and $\lfloor n/2 \rfloor + 1$ respectively. Let $M_n = A_n \cup B_n \cup C_n$, then $|M_n| = (3 + o(1))N$. Given a subset G_n of M_n, define

$$\rho(G_n) = \frac{|G_n \cap A_n|}{|A_n|} + \frac{|G_n \cap B_n|}{|B_n|} + \frac{|G_n \cap C_n|}{|C_n|}.$$

In the following we view a family of subsets as its Hasse diagram. This allows us to talk about subsets as vertices and edges for subsets that differ by exactly one element. Let $\mathcal{H}_n$ be the family of all Q_2-free subsets of M_n, then we can write the result in [2] as

$$\lim_{n\to\infty} \max_{G_n \in \mathcal{H}_n} \{\rho(G_n)\} \leq (3+\sqrt{2})/2.$$

The same result can be achieved by considering $\mathcal{H}_2$ (see Figure 7), and two flags (see Figure 8). An additional constraint for the flags is that the labeled vertex is from A_n or C_n, and the unlabeled vertex is from B_n. A black vertex indicates that the corresponding subset of $[n]$ is present in the subposet and a white vertex indicates the opposite.

Given $G_n \in \mathcal{H}_n$, let $p(H_i, G_n)$ be the probability that a random subset $D \simeq Q_2$ of M_n chosen uniformly at random satisfies $D \cap G_n \simeq H_i$, then

$$\rho(G_n) = \sum_i \rho(H_i) p(H_i, G_n).$$

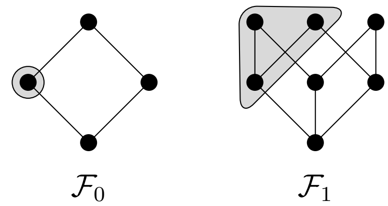

Figure 9: Flags families used in the computer assited proof.

For the flags, for a vertex θ in $A_n \cup C_n$, we define $p(F_i, \theta, G_n)$ to be the probability that a random vertex v from B_n that is adjacent to θ (i.e. the set corresponding to v contains the set corresponding to θ or is in θ) satisfies $\{\theta, v\} \simeq F_i$. We also define $p(F_i, F_j, \theta, G_n)$ to be the probability that two random vertices $u \neq v$ from B_n that are adjacent to θ satisfy $\{\theta, u\} \simeq F_i$ and $\{\theta, v\} \simeq F_j$. A lemma analogous to Lemma 2 can be proven, we omit the details. Hence we can apply flag algebra method to this setup and get Table 2.

	H_0	H_1	H_2	H_3	H_4	H_5	H_6	H_7	H_8	H_9	H_{10}
ρ	0	1	1	1/2	1	3/2	3/2	2	5/2	2	2
F_0, F_0	0	1/2	1/2	0	0	0	0	1	0	0	0
F_0, F_1	0	0	0	0	0	1/4	1/4	0	1/2	0	0
F_1, F_1	0	0	0	0	0	0	0	0	0	1/2	1/2

Table 2: $\rho(H_k)$ and $\mathbb{E}_\theta p(F_i, F_j, \theta, H_k)$.

Then a semidefinite matrix

$$M = \begin{pmatrix} \frac{\sqrt{2}-1}{2} & \frac{\sqrt{2}-2}{2} \\ \frac{\sqrt{2}-2}{2} & \sqrt{2}-1 \end{pmatrix}$$

gives the desired bound $\frac{3+\sqrt{2}}{2}$.

The proof of Theorem 3 goes along the same lines as for $\frac{3+\sqrt{2}}{2}$. One difference is that three middle layers of Q_4 are considered instead of Q_2. The number of Q_2-free subgraphs is 606. The other difference is that we use flag families depicted in Figure 9. Each family contains flags obtained from the depicted ones by coloring the vertices black and white. Sources of a program for generating Q_2-free subgraphs and computing an analog of Table 2 are available at `http://www.math.uiuc.edu/~jobal/cikk/hypercube`.

7 Conclusion

We presented an adaptation of Razborov's flag algebra method to subgraphs of the hypercube. Using the adaptation we obtained new upper bounds on densities in limit on 4-cycle and 6-cycle free subgraphs of the hypercube.

We suspect that the method can give a better bound when applied to the hypercubes of dimension greater than 3. However, we found 3212821 C_4-free spanning subgraphs of $\mathcal{Q}_4$. The resulting semidefinite program is currently too large for CSDP.

We were trying to reduce the number of considered C_4-free subgraphs by identifying those with the same $\rho(H) + c_H$. The only set of flags we discovered that was leading to a solvable semidefinite program was consisting of flags whose vertices induce a star in the hypercube. See F_1 in Figure 2 for an example. In this setting $\rho(H_1) + c_{H_1} = \rho(H_2) + c_{H_2}$ if C_4-free spanning subgraphs H_1 and H_2 have the same degree sequence. Unfortunately, the resulting bounds were worse than the bounds obtained from $\mathcal{Q}_3$ and square like flags.

Maybe a good set of flags, a better solver or just some future hardware can make such problems solvable.

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